The 4-spinon dynamical structure factor of the Heisenberg chain

Jean-Sébastien Caux and Rob Hagemans

Institute for Theoretical Physics, University of Amsterdam, 1018 XE Amsterdam, The Netherlands.

Abstract. We compute the exact 4-spinon contribution to the zero-temperature dynamical structure factor of the spin-1/2 Heisenberg isotropic antiferromagnet in zero magnetic field, directly in the thermodynamic limit. We make use of the expressions for matrix elements of local spin operators obtained by Jimbo and Miwa using the quantum affine symmetry of the model, and of their adaptation to the isotropic case by Abada, Bougourzi and Si-Lakhal (correcting some overall factors). The 4-spinon contribution to the first frequency moment sum rule at fixed momentum is calculated. This shows, as expected, that most of the remaining correlation weight above the known 2-spinon part is carried by 4-spinon states. Our results therefore provide an extremely accurate description of the exact structure factor.

1. Introduction

It has now been 75 years since Hans Bethe published his seminal paper [1] constructing the eigenfunctions of the spin-1/2 Heisenberg chain [2],

$$H = \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \tag{1}$$

giving birth to the Bethe Ansatz and paving the way for the modern theory of integrable models of quantum mechanics and field theory [3, 4, 5]. Interest in the Heisenberg model has only increased since those early days, partly because of the extremely rich mathematical structures now known to be associated to it, but also because of its ability to accurately describe a number of real compounds.

The Bethe Ansatz is first and foremost a method giving access to an integrable system's energy levels, allowing the calculation of many equilibrium quantities. For the specific case of the Heisenberg model, the ground state energy of the infinite chain was computed analytically [6] not long after Bethe's paper, but it was not until the 1960's that significant new results were obtained: its excitation spectrum was computed by des Cloizeaux and Pearson [7], and its more general thermodynamic properties were obtained shortly afterwards [8, 9, 10, 11].

Equilibrium quantities are however not sufficient to completely characterize the physics of models such as (1). Motivated mainly by experimental work, another object of fundamental importance has been extensively studied: the dynamical structure factor (DSF)

$$S^{ab}(k,\omega) = \sum_{l=1}^{N} e^{ikl} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S^a_{j+l}(t) S^b_j(0) \rangle, \qquad \text{a,b = x, y, z.} \tag{2}$$

This quantity is directly accessible experimentally through inelastic neutron scattering [12, 13, 14, 15], and its theoretical calculation opens the door to the interpretation of a wealth of experimental data.

Despite much effort, the dynamics of integrable models remains in general inaccessible, and exact calculations based on the Bethe Ansatz can only rarely be carried out. One reason is that excitations are usually rather complicated: for the Heisenberg model, the Hilbert space can be spanned with spinons [16, 17, 18], which are nontrivially interacting spin-1/2 particles whose dispersion relation is given by

$$e(p) = \frac{\pi}{2} |\sin p|, \qquad p \in [-\pi, 0]. \tag{3}$$

The computation of dynamical quantities such as the structure factor however requires knowledge of matrix elements of spin operators between (multi-)spinon states, which goes much beyond what is accessible with the basic Bethe Ansatz.

In view of the difficulty of this task, a number of approximate schemes have been put forward to offer a qualitative picture of the DSF. One extremely useful construction is known as the Müller ansatz [19], which is based on exact results for the XY model, numerical computations on small chains and known sum rules. Its success lies in its extreme simplicity, coupled with rather accurate reproduction of a number of features (like the square-root singularity at the lower threshold). It is commonly used in the interpretation of experimental data. It drawback is that it is inexact; in particular, its functional form at the top of the 2-spinon continuum is not correct.

Another important and successful approach relies on mapping the infinite chain onto a relativistic quantum field theory [20, 21]. Finite size scaling connects the critial exponents of the system with its behaviour in a finite volume [22, 23], while conformal field theory [24, 25] and bosonization allow the calculation of asymptotics of correlation functions [26, 27, 28] even at finite temperatures, with known normalizations for the first few leading terms in the operator expansion [29, 30, 31].

As far as methods based on integrability are concerned, it is now possible to achieve extremely accurate computations of the DSF over the whole Brillouin zone [32, 33] for integrable Heisenberg spin chains of any anisotropy in any magnetic field, using the ABACUS method [34]. These computations rely on determinant representations for matrix elements of local spin operators obtained by solving the quantum inverse problem [35, 36], and are therefore limited to finite (albeit large) chains. We here wish however to concentrate on an altogether different and independent take on the problem of calculating the DSF of the Heisenberg model, which is not applicable in general but only in one particular (albeit extremely important) case.

The crucial development (as far as the subject of the present paper is concerned) came with the recognition that the infinite chain in zero magnetic field displayed a quantum affine symmetry, allowing the diagonalization of the Hamiltonian directly in the thermodynamic limit [37]. Multi-spinon states then provide a basis for the Hilbert space and a resolution of the identity operator, allowing to write the DSF as a sum of matrix elements of local spin operators. These matrix elements can be computed within this framework through bosonization of the quantum affine algebra [38, 39, 40], a task performed by Jimbo and Miwa [41]. The general representation of such correlation functions as the DSF is then obtained in terms of rather complicated contour integrals, the number of integrals increasing with the number of spinons in the excited state. These are however notoriously hard to evaluate quantitatively.

One exception is the contribution to the transverse zero-temperature DSF of the Heisenberg model coming from 2-spinon intermediate states, the simplest excitations that can be constructed above the ground state. In this case, the dynamical constraints of conservation of energy and momentum give two δ functions taking care of the two contour integrals involved, allowing for a direct analytical calculation [42] (a similar calculation is also possible in the whole gapped antiferromagnetic phase [43]). These 2-spinon intermediate states were shown to contribute 72.89% of the total structure factor intensity [44]. The missing part is then necessarily carried by excited states with a higher number of spinons, starting with 4-spinon states.

The integral representations for matrix elements involving 4-spinon states are much more difficult to tackle, since the dynamical constraints are not sufficient to take care of all the contour integrals involved (this is also true for the longitudinal structure factor of the XXZ model, which was studied in the Ising limit in [45]). The first attempt to tackle more than two spinons was made in [46], offering a formal representation for the exact n-spinon contribution for the zero-temperature DSF of the Heisenberg model in zero field. A more thorough treatment of the four-spinon case was published shortly afterwards [47], yielding expressions for the DSF in the whole gapped antiferromagnetic regime, and their specialization to the Ising and Heisenberg limits. These expressions remained however quite complicated, giving the four-spinon part at fixed momentum and energy in terms of a double integral of an infinite series. Further analytical work [48] yielded little progress, and in fact (as we will show below) incorrectly identified the boundaries of the four-spinon continuum. To this

day, nobody has been able to extract curves from these expressions, and previous attempts [49, 50] have not yielded acceptable results due to the inappropriateness of the chosen method and the incorrect continuum used.

The present paper offers the first reliable computation of the exact 4-spinon contribution to the zero-temperature dynamical structure factor of the Heisenberg isotropic antiferromagnet in zero magnetic field. After summarizing results for the matrix elements which we need for our purposes, the known 2-spinon results are repeated as a warmup, after which we present their extension to the case of four spinons (correcting some factors in the formulas present in the literature). We finish by a discussion of our results, in particular concerning contributions to sum rules.

2. Exact representation of the dynamical structure factor

The inevitable first step in the calculation of the DSF (2) is to insert a resolution of the identity in a judiciously chosen basis between the two spin operators. For the XXZ model in the thermodynamic limit, a basis for the Hilbert space is provided by (multi-) spinon states $|\xi_1, ..., \xi_n\rangle_{\epsilon_1,...,\epsilon_n;i}$, which diagonalize the Hamiltonian according to

$$H|\xi_1, ..., \xi_n\rangle_{\epsilon_1,...,\epsilon_n;i} = \sum_{j=1}^{n} e(\xi_j)|\xi_1, ..., \xi_n\rangle_{\epsilon_1,...,\epsilon_n;i} \tag{4}$$

where i labels the two equivalent vacuum states $|0\rangle_i$, $i = 0, 1$ corresponding to the two different possible boundary conditions, and $\epsilon_i = \pm 1$ labels the spin projection of the spinons. The coefficients ξ_j are spectral parameters determining the energy and momenta of the spinons. The completeness relation reads

$$\mathbf{1} = \sum_{i=0,1} \sum_{n\geq 0} \sum_{\epsilon_1,...,\epsilon_n=\pm 1} \frac{1}{n!} \oint \prod_{j=1}^{n} \frac{d\xi_j}{2\pi i \xi_j} |\xi_n, ..., \xi_1\rangle_{\epsilon_n,...,\epsilon_1;i} \; {}_{i;\epsilon_1,...,\epsilon_n}\langle \xi_1, ..., \xi_n| \tag{5}$$

and can be substituted in (2) to yield the decomposition of the DSF into a sum over (even numbers of) spinon contributions (here and in the following, we make use of spin isotropy and compute $S(k, \omega) \equiv S^{zz}(k, \omega) = S^{xx} = S^{yy}$)

$$S(k, \omega) = \sum_{n \ even} S_n(k, \omega). \tag{6}$$

Each term in this decomposition is explicitly written as

$$S_n(k, \omega) = \frac{2\pi}{n!} \sum_{m\in \mathbf{Z}} \sum_{\epsilon_1,...,\epsilon_n=\pm 1} \oint \prod_{j=1}^{n} \frac{d\xi_j}{2\pi i \xi_j} e^{im(k+\sum_{j=1}^{n} p_j)} \delta(\omega - \sum_{j=1}^{n} e_j) \times$$
$$\times {}_i\langle |0|S_0^z(0)|\xi_n, ..., \xi_1\rangle_{\epsilon_n,...,\epsilon_1;i} \; {}_{i;\epsilon_1,...,\epsilon_n}\langle \xi_1, ..., \xi_n|S_0^z(0)|0\rangle_i. \tag{7}$$

The matrix elements of local spin operators in the above expression are represented exactly within the framework of Jimbo and Miwa [41]. Their adaptation to the isotropic Heisenberg antiferromagnet was given in [42] for 2-spinon intermediate states, and in [46] for $n > 2$, although the expressions obtained there are not thoroughly simplified. For 4-spinon intermediate states, the matrix elements were studied more extensively in [47], whose results will form the basis of the new results we obtain. Let us however start by briefly reminding the reader of known results on the much simpler case of 2-spinon intermediate states.

3. 2-spinon contribution to the structure factor

It is well-known that 2-spinon intermediate states live within a continuum in k, ω defined by satisfying the kinematic constraints of momentum and energy conservation,

$$k = -p_1 - p_2, \qquad \omega = e(p_1) + e(p_2). \tag{8}$$

In other words, for a fixed external momentum, there exists an interval in frequency given by the conditions

$$\omega \geq \omega_{2,l}(k) = \frac{\pi}{2}|\sin k|, \qquad \omega \leq \omega_{2,u}(k) = \pi \sin\frac{k}{2}, \qquad k \in [0, 2\pi]. \tag{9}$$

The lower boundary is thus given by the des Cloizeaux-Pearson dispersion relation. The 2-spinon part of the DSF will be nonvanishing within this continuum, and will by construction vanish identically outside of it. This contribution was obtained in [42] and is explicitly written as

$$S_2(k,\omega) = \frac{1}{2}\frac{e^{-I(\rho(k,\omega))}}{\sqrt{\omega_{2,u}^2(k) - \omega^2}}\Theta(\omega_{2,u}(k) - \omega)\Theta(\omega - \omega_{2,l}(k)). \tag{10}$$

The parameter ρ is defined as

$$\cosh(\pi\rho(k,\omega)) = \sqrt{\frac{\omega_{2,u}^2(k) - \omega_{2,l}^2(k)}{\omega^2 - \omega_{2,l}^2(k)}} \tag{11}$$

and the nontrivial part of the DSF is encoded in the fundamental integral function

$$I(\rho) = \int_0^\infty dt \frac{e^t}{t}\frac{\cosh(2t)\cos(4\rho t) - 1}{\cosh t \sinh(2t)}. \tag{12}$$

A careful study of this representation of the 2-spinon DSF was carried out in [44], and it is worthwhile to remind the reader of some important facts obtained there. First of all, at the lower boundary (for $q \neq \pi$), the 2-spinon DSF diverges as a square root accompanied by a logarithmic correction, $S_2 \sim \frac{1}{\sqrt{\omega - \omega_{2,l}(k)}}\sqrt{\ln\frac{1}{\omega - \omega_{2,l}(k)}}$ (for $q = \pi$, the divergence is $\sim \frac{1}{\omega}\sqrt{\ln\frac{1}{\omega}}$). Near the upper boundary, on the other hand, the 2-spinon DSF vanishes in a square-root cusp, $S_2 \sim \sqrt{\omega_{2,u}(k) - \omega}$.

Second, sum rules were also studied, most importantly the contribution to the total integrated intensity

$$\int_0^{2\pi}\frac{dk}{2\pi}\int_0^\infty \frac{d\omega}{2\pi} S(k,\omega) = \frac{1}{4} \tag{13}$$

and to the exactly known first frequency moment at fixed momentum,

$$K_1(k) = \int_0^\infty \frac{d\omega}{2\pi}\omega S(k,\omega) = (1 - \cos k)\frac{2e_0}{3} \tag{14}$$

where $e_0 = 1/4 - \ln 2$ is the ground-state energy density [6]. 2-spinon intermediate states were shown to carry 72.89% of the total intensity, and 71.30% of the first moment sum rule (independently of k).

More than a quarter of the exact DSF is therefore missing if we restrict ourselves to only two spinons. To achieve better saturation of the sum rules, we need to go to more complicated intermediate states involving more particles, and we can safely expect that out of those, 4-spinon states will be dominant.

4. 4-spinon contribution to the structure factor

Starting from the results of [47], we write the exact representation for the 4-spinon part of the DSF as

$$S_4(k,\omega) = C_4 \int_{-\pi}^{0} dp_1 ... dp_4 \;\; \delta_{(2\pi)}(k + \sum_i p_i) \;\; \delta(\omega + \sum_i e(p_i)) \;\; J(\{p\}) \tag{15}$$

where the prefactor is

$$C_4 = \frac{1}{3 \times 2^9} \frac{1}{\Gamma(1/4)^8 |A(i\pi/2)|^8}, \tag{16}$$

with

$$A(z) = \exp\left(- \int_0^\infty dt \frac{e^t}{t} \frac{\sinh^2(t[1 + i\frac{z}{\pi}])}{\sinh(2t)\cosh t} \right). \tag{17}$$

Here again, we restrict to $k \in [0, \pi]$. Parametrizing the momenta as

$$\cot p_i = \sinh(2\pi\rho_i) \tag{18}$$

the correlation weight is explicitly given by

$$J(\{p\}) \equiv J(\{\rho\}) = e^{-\sum_{1 \le i < j \le 4} I(\rho_{ij})} \sum_{l=1}^{4} |g_l(\{\rho\})|^2 \tag{19}$$

where $\rho_{ij} = \rho_i - \rho_j$. The function $I(\rho)$ is given by equation (12), whereas g_l is given by the following expression:

$$g_l = (-1)^{l+1} \sum_{j=1}^{4} \cosh(2\pi\rho_j) \times$$

$$\times \sum_{m=\Theta(j-l)}^{\infty} \frac{\prod_{i \neq l}(m - \frac{1}{2}\Theta(l-i) + i\rho_{ji})}{\prod_{i \neq j} \sinh(\pi\rho_{ji})} \prod_{i=1}^{4} \frac{\Gamma(m - \frac{1}{2} + i\rho_{ji})}{\Gamma(m + 1 + i\rho_{ji})} \tag{20}$$

where the Heaviside function is here defined as $\Theta(n) = 0$ for $n \le 0$ and $\Theta(n) = 1$ for $n > 0$.

We have corrected two inaccuracies in [47]: first, the correct normalization is presented here (compare (20) with formula (5.10) there), and most importantly, we have explicitly written that the momentum δ function fixes k only modulo 2π. This has the crucial consequence that two sectors must be considered when solving the dynamical constraints of momentum and energy conservation for 4-spinon intermediate states (this was overlooked in [48, 49, 50], leading in particular to an incorrect description of the four-spinon continuum). Bearing in mind that the spinon momenta p_i are by definition constrained to the interval $[-\pi, 0]$, we define sectors 0 and 1 as

$$0 : k + p_1 + p_2 + p_3 + p_4 = 0, \qquad 1 : k + 2\pi + p_1 + p_2 + p_3 + p_4 = 0 \tag{21}$$

with in both cases the energy constraint explicitly written as

$$\omega + \frac{\pi}{2}(\sin p_1 + \sin p_2 + \sin p_3 + \sin p_4) = 0. \tag{22}$$

For higher spinon numbers, more sectors must be similarly added: there are n such sectors for states with $2n$ spinons.

A more physical representation of the four-spinon part (15) of the structure factor is obtained by the change of variables $\{p_i\} \to \{k, \omega, K, \Omega\}$ where

$$K = -p_1 - p_2, \qquad \Omega = -\frac{\pi}{2}(\sin p_1 + \sin p_2). \tag{23}$$

In sector 0, we then have

$$K = k + p_3 + p_4, \qquad \Omega = \omega + \frac{\pi}{2}(\sin p_3 + \sin p_4). \tag{24}$$

The complete transformation reads

$$p_1 = -\frac{K}{2} + \mathrm{acos}\frac{\Omega}{\omega_{2,u}(K)}, \qquad p_2 = -\frac{K}{2} - \mathrm{acos}\frac{\Omega}{\omega_{2,u}(K)},$$
$$p_3 = \frac{K-k}{2} + \mathrm{acos}\frac{\omega - \Omega}{\omega_{2,u}(k-K)}, \qquad p_4 = \frac{K-k}{2} - \mathrm{acos}\frac{\omega - \Omega}{\omega_{2,u}(k-K)}, \tag{25}$$

where we restrict to $p_1 > p_2$ and $p_3 > p_4$ by symmetry. This sector corresponds to $K \in [0, k]$.

In sector 1, we have

$$K = k + 2\pi + p_3 + p_4 \tag{26}$$

instead of the left of (24), yielding the same expressions for p_1 and p_2, and

$$p_3 = -\pi + \frac{K-k}{2} + \mathrm{acos}\frac{\omega - \Omega}{\omega_{2,u}(K-k)}, \quad p_4 = -\pi + \frac{K-k}{2} - \mathrm{acos}\frac{\omega - \Omega}{\omega_{2,u}(K-k)}, \tag{27}$$

with the same restrictions as above. This sector corresponds to $K \in [k, 2\pi]$.

The 4-spinon continuum in the k, ω plane is obtained by letting K and Ω take on all their allowed values. The lower boundary coincides with that of the 2-spinon continuum (the des Cloizeaux-Pearson dispersion relation; this is clearly the case from a simple physical argument, namely that we are dealing with a massless theory, and therefore adding two more spinons of zero momentum in the intermediate state does not shift the energy; in fact, the lower boundary of *any* finite higher spinon number continuum is identical to the 2-spinon one). The upper boundary, on the other hand, extends above the upper boundary of the 2-spinon continuum, and is obtained by sharing the momentum (modulo 2π) evenly among the four spinons. Explicitly, we therefore have

$$\omega_{4,l}(k) = \omega_{2,l}(k) = \frac{\pi}{2}|\sin k|, \qquad \omega_{4,u}(k) = \pi\sqrt{2\left(1 + |\cos\frac{k}{2}|\right)}. \tag{28}$$

A geometrical picture of the $2n$ spinon continuum is easily obtained by generalization: the lower boundary will always be given by the des Cloizeaux-Pearson dispersion relation, whereas the upper boundary will be given by the upper boundary of a 2-spinon continuum rescaled in size by a factor of n, modulo all its 2π translations (refer to Figure 2 for the simplest case of 4 spinons).

For the implementation of the computation of the 4-spinon part of the structure factor, it is desirable to describe more carefully the actual integration regions for K and Ω, which can be precisely defined for given $k \in [0, \pi]$ and $\omega \in [\omega_{4,l}(k), \omega_{4,u}(k)]$. Simple reasoning shows that the K, Ω integration regions are obtained by intersecting two separate 2-spinon continua, one upright and the other inverted in frequency, and shifted with respect to each other by k in momentum and ω in frequency (this is illustrated in Figure 1). The important line crossings are respectively of the $\omega_{2,u}$ lines (upper boundaries) of the two continua, and of their $\omega_{2,l}$ lines. The first determine

which intervals of K should be included, and the second determine which sub-intervals within these should be excluded.

Regions of K to be included depend on the values of k and ω, and are given by

$$\begin{aligned} &\omega \leq \pi \sin \frac{k}{2} : && K \in [0, 2\pi] \\ &\pi \sin \frac{k}{2} < \omega \leq 2\pi \sin \frac{k}{4} : && K \in [K_{1a}^-, K_{1a}^+] \cup [K_{1b}^-, K_{1b}^+] \end{aligned} \tag{29}$$

where

$$K_{1a}^{\pm} = \frac{k}{2} + \pi \pm 2\text{acos}\frac{\omega}{2\pi \cos \frac{k}{4}}, \qquad K_{1b}^{\pm} = \frac{k}{2} \pm 2\text{acos}\frac{\omega}{2\pi \sin \frac{k}{4}}. \tag{30}$$

The lower boundaries of the intersecting continua define excluded regions of K as

$$\begin{aligned} &\frac{\pi}{2} \sin k \leq \omega \leq \pi \sin \frac{k}{2} : && K \notin [K_{2c}^-, K_{2c}^+] \cup [K_{2c}^- + \pi, K_{2c}^+ + \pi], \\ &\frac{\pi}{2} \sin k \leq \omega \leq \pi \cos \frac{k}{2} : && K \notin [K_{2d}^-, K_{2d}^+] \cup [K_{2d}^- + \pi, K_{2d}^+ + \pi] \end{aligned} \tag{31}$$

where

$$K_{2c}^{\pm} = \frac{k}{2} + \frac{\pi}{2} \pm \text{acos}\frac{\omega}{\pi \cos \frac{k}{2}}, \qquad K_{2d}^{\pm} = \frac{k}{2} \pm \text{acos}\frac{\omega}{\pi \sin \frac{k}{2}}. \tag{32}$$

We define the K integration domain $\mathcal{D}_K$ as the sum of (possibly disconnected) regions fulfilling the above constraints.

For fixed k, ω, K fulfilling the above constraints, the value of Ω is restricted to a finite interval:

$$\Omega_l(k, \omega, K) \leq \Omega \leq \Omega_u(k, \omega, K), \tag{33}$$

with the limits being explicitly given by

$$\begin{aligned} \Omega_l(k, \omega, K) &= \text{Max}\left(\frac{\pi}{2}|\sin K|, \omega - \pi \sin |\frac{k-K}{2}|\right), \\ \Omega_u(k, \omega, K) &= \text{Min}\left(\pi \sin \frac{K}{2}, \omega - \frac{\pi}{2}|\sin(k-K)|\right). \end{aligned} \tag{34}$$

The leftover two-dimensional integral for the 4-spinon part of the DSF is therefore over a region with nontrivial geometry, depending on the particular values of k and ω. Within the 4-spinon continuum, we can identify six sectors (illustrated in Figure 2), each of which leads to a different sort of integration domain in the K, Ω plane (examples of which are illustrated in Figure 4). By symmetry, we only need to consider $k \in [0, \pi]$.

In terms of the new variables k, ω, K, Ω, the kinematic restrictions are trivially implemented, and the four-spinon contribution to the structure factor can be written as a two-dimensional integral in K and Ω over the regions defined above:

$$S_4(k, \omega) = C_4 \int_{\mathcal{D}_K} dK \int_{\Omega_l(k,\omega,K)}^{\Omega_u(k,\omega,K)} d\Omega \, \frac{J(k, \omega, K, \Omega)}{\left\{\left[\omega_{2,u}^2(K) - \Omega^2\right]\left[\omega_{2,u}^2(k-K) - (\omega - \Omega)^2\right]\right\}^{1/2}} \tag{35}$$

where we have written J implicitly as a function of the new variables.

For the evaluation of this expression, we use a specially adapted Romberg-like integration method. The integrand typically has integrable divergences at the boundaries of the integration regions, which are absorbed by various appropriate changes of variables before coding. While technically feasible as we demonstrate

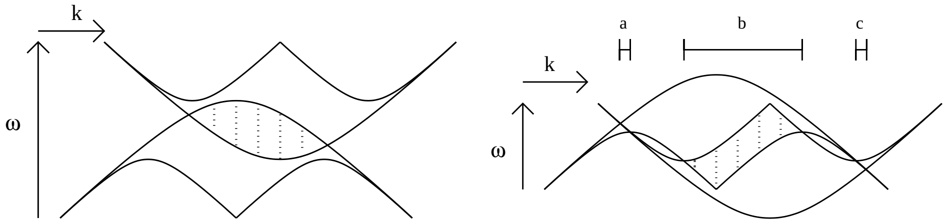

Figure 1. Integral regions in the K, Ω plane. These are formed by the intersection of two 2-spinon continua, one of them inverted, and shifted with respect to one another by k and ω. The left-hand example is a simple case where only one connected domain is obtained. On the right is a more complicated example with three different integration domains (whose K borders are pointed out above; the domains delimited by a and c have a very small but finite area).

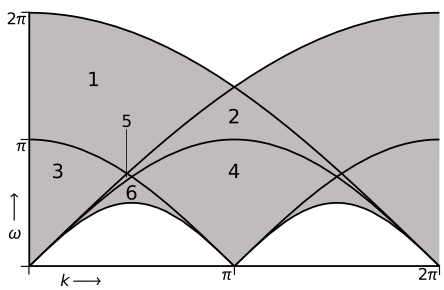

Figure 2. For values of k and ω within the 4-spinon continuum (shaded), the K and Ω integration regions take different forms. Six sectors are obtained, as labeled here (sector 5 is barely visible, bordered by sectors $2, 3, 6$). Examples of K, Ω integration regions for each of these sectors are given in Figure 4.

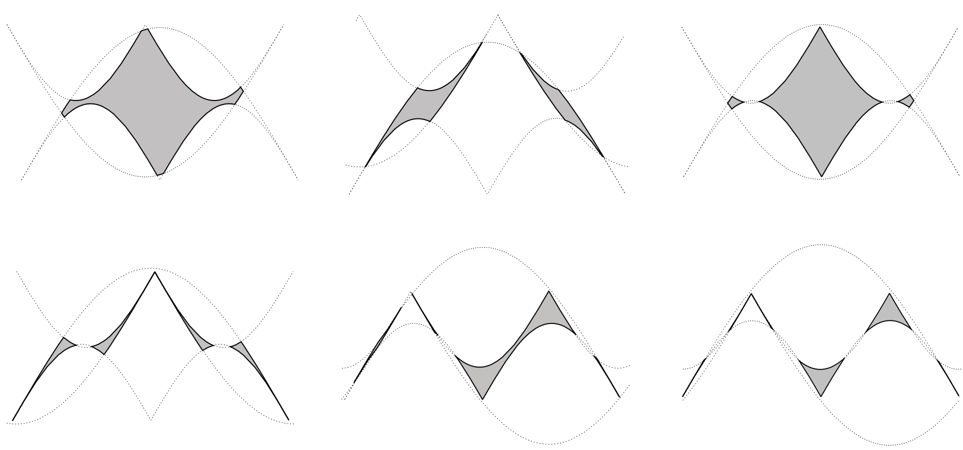

Figure 3. Integration domains in the K, Ω plane (shaded) for the six sectors given in Figure 2 ($1-3$ top left to right, $4-6$ bottom). The $K = 0, \Omega = 0$ origin always lies at the left foot of the upright 2-spinon continuum.

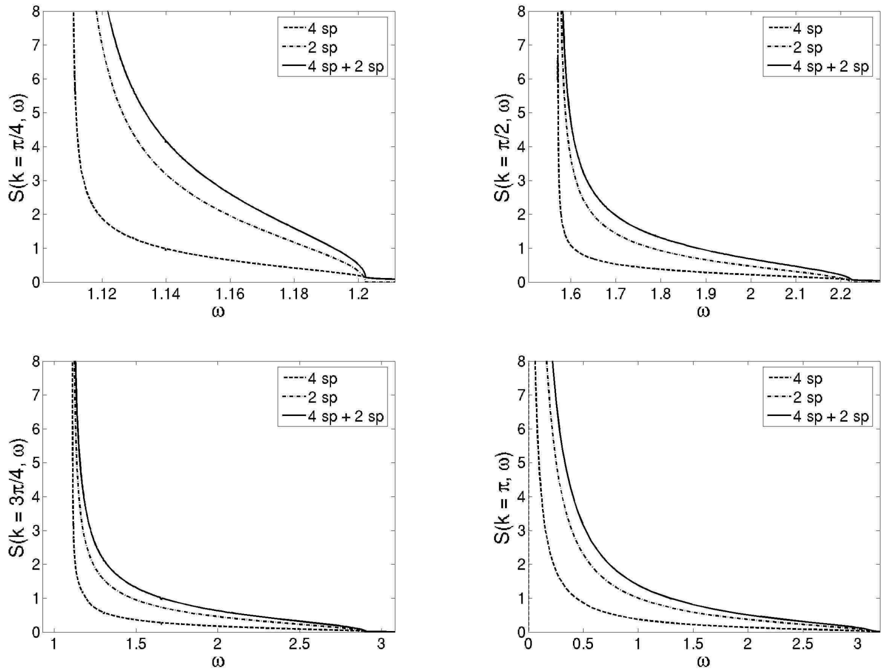

Figure 4. Plots of the 2- and 4-spinon parts of the dynamical structure factor at momenta $k = \pi/4, \pi/2, 3\pi/4$ and π. The horizontal axis is frequency, and we focus on the region of the 2-spinon continuum for ease of comparison.

here, it remains a challenge to obtain very good precision, and we therefore here first concentrate on results for fixed momentum.

The main results are plotted in Figure 4, for four representative values of k (other values give similar-looking plots). Over the 2-spinon continuum, the 4-spinon contribution is of the same order as the 2-spinon one (*i.e.* about a third of it). Between the upper boundary $\omega_{2,u}$ of the 2-spinon continuum and the upper boundary $\omega_{4,u}$ of the 4-spinon continuum, the 4-spinon part of the structure factor is finite but very small. Figure 5 displays the shape of the DSF in the vicinity of the 2-spinon upper boundary for two representative values of momentum (the same sort of behaviour is observed for all momentum values we checked). A few things are worth pointing out here. First, at the lower boundary, the 4-spinon part diverges similarly to the 2-spinon one. Second, the 4-spinon part is finite and smooth around the upper boundary $\omega_{2,u}$ of the 2-spinon continuum. The full DSF therefore still has a square-root singularity around this point, yielding a picture consistent with that put forward in [51] (see also the related discussion in [52]). At higher frequencies, the DSF decays extremely rapidly, as illustrated in Figure 6.

To assess the quality of our results at fixed momentum, we compute the first frequency moment sum rule in Table 1. 4-spinon intermediate states clearly carry (as expected) the majority of the missing correlation weight after 2-spinon contributions have been taken into account, *i.e.* around 27% $\pm 1\%$ of this sum rule for all values of momentum which were studied. We have not yet achieved sufficient accuracy for the 4-spinon part of the total integrated intensity, but we can expect again a

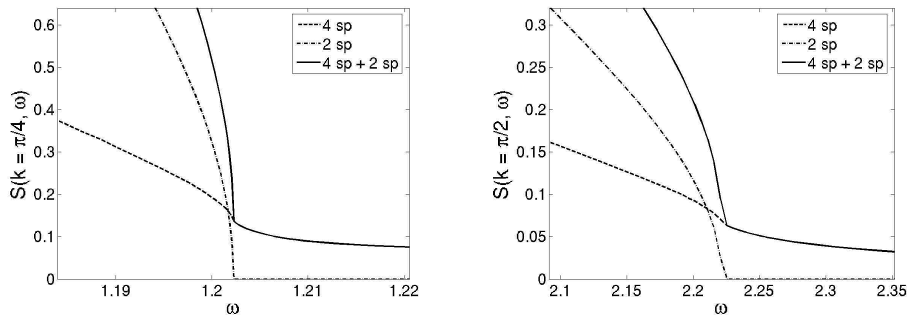

Figure 5. Zooms on the upper boundary of the 2-spinon continuum, here for $k = \pi/4$ and $\pi/2$ (other values of momentum give very similar results). The 2-spinon part vanishes in a square root cusp at $\omega_{2,u}$, whereas the 4-spinon part is finite. There is thus an infinite slope in the full dynamical structure factor at $\omega_{2,u}$.

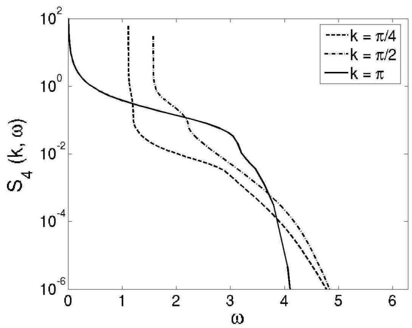

Figure 6. The 4-spinon part (in logarithmic scale) of the DSF as a function of frequency for three representative values of momentum. The upper boundary of the 2-spinon continuum is visible as the shoulder in the curve, with the 4-spinon part of the DSF decreasing rapidly above this threshold.

k	$\pi/8$	$\pi/4$	$3\pi/8$	$\pi/2$	$5\pi/8$	$3\pi/4$	$7\pi/8$	π
$K_1(k)$ (4 sp %)	27.2	27.3	27.3	27.1	26.5	26.2	25.9	26.6

Table 1. First frequency moment sum rule (see equation (14)) percentages coming from the 4-spinon part of the dynamical structure factor. The 2-spinon part always contributes 71.30%. 4-spinon states clearly carry the majority of the leftover correlation weight, as is naturally expected. The accuracy of these results is estimated to be around 1% of $K_1(k)$.

contribution of the order of 27% (since the general shape of the 4-spinon part resembles that of the 2-spinon part, and since the relative 2-spinon part of both sum rules is almost equal). There thus remains only about 2% missing, which are naturally ascribed to higher spinon numbers. Although these are also in principle accessible using an extension of the present method, the (for 6 spinons, quadruple) integrations needed probably prohibit accurate evaluation without first achieving significant further analytical advances. However, this missing part is now rather small, meaning that our results provide an approximation of the exact zero-temperature DSF of the Heisenberg model in zero field which is the most accurate available at the moment.

Conclusion

In conclusion, we have calculated the 4-spinon contribution to the zero-temperature dynamical structure factor of the Heisenberg model in zero magnetic field, starting from its exact integral representation in the thermodynamic limit. As proven by sum rules, this contribution carries most of the correlation weight left over after 2-spinon intermediate states have been taken into accout. The results obtained therefore provide a very close description of the exact correlator. In future publications, we will provide a thorough analysis of other available sum rules, and extend the results to the gapped antiferromagnetic case.

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